2-(propan-2-yl)-1,3,6-trioxocane

15351-38-9 | DTXSID80279934

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 196 °C

Global applicability domain: Inside

Local applicability domain index: 7.18e-01

Confidence level: 8.61e-01

Nearest Neighbors from the Training Set

Image not found
Butyl dichloroacetate
Measured: 194
Predicted: 188

Image not found
2-Butoxyethyl acetate
Measured: 192
Predicted: 191

Image not found
Cyclohexanecarboxylic acid, ethyl ester
Measured: 196
Predicted: 196

Image not found
Cyclohexyl propionate
Measured: 193
Predicted: 196